

EES Catalysis

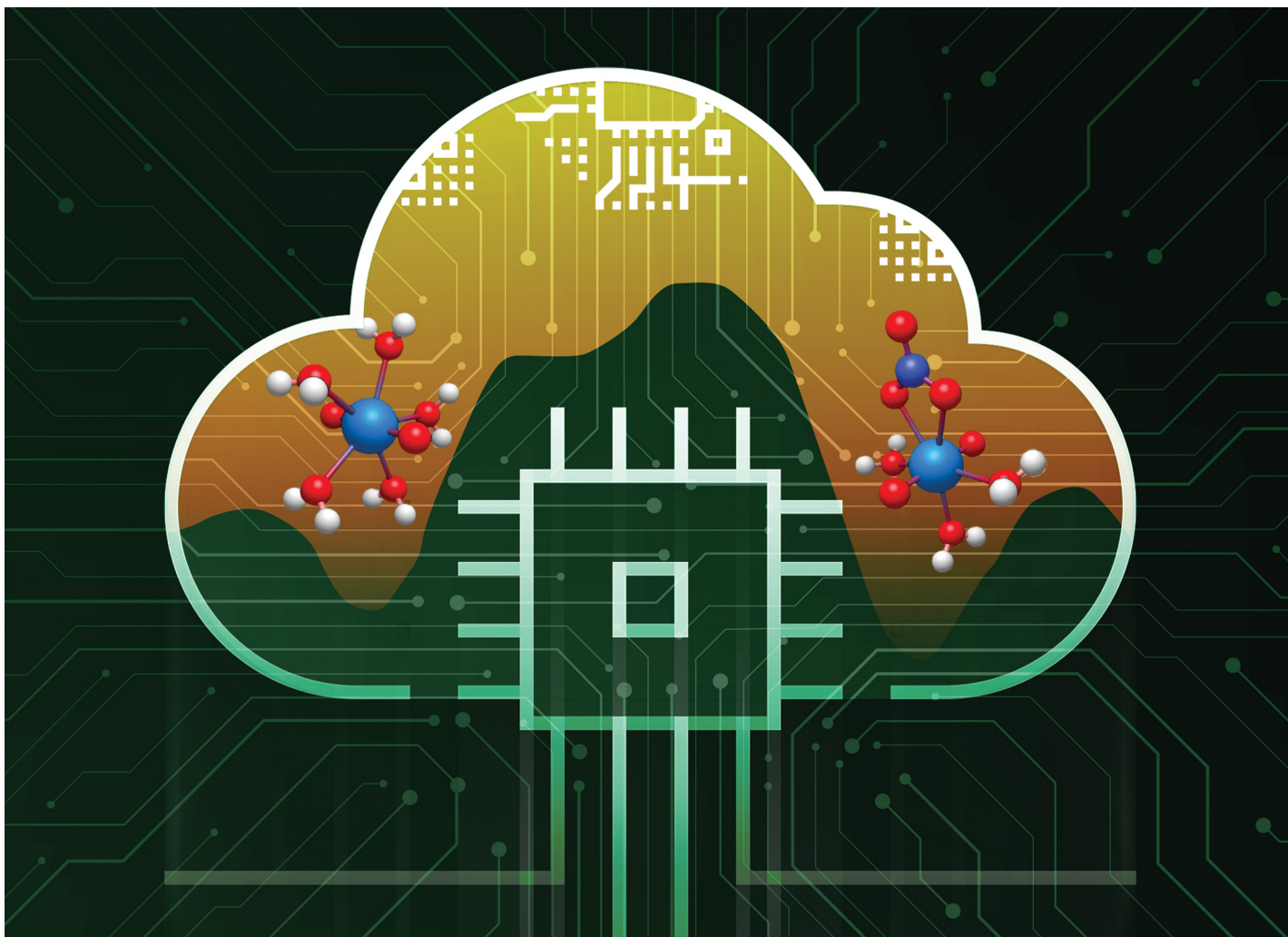
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Fundamental questions
Elemental answers



Showcasing research from the Generative AI for Science, Energy, and Security Science & Technology Investment at Pacific Northwest National Laboratory, USA.

On the stability constants of metal-nitrate complexes in aqueous solutions

This work uses a cloud computational framework to determine ligand-exchange reaction-free energies and coordination chemistry of alkaline earth, transition, actinide, and lanthanide metal complexes at quantum-level accuracy. It provides new physico-chemical insights about monodentate-bidentate competition in metal-nitrate complexes for Generative-AI-based multiscale modelling of ion coordination, speciation relevant to separations processes in nuclear forensics.

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As featured in:



See Mohammadhasan Dinpajoo, Nicolas E. Uhnak *et al.*, *Phys. Chem. Chem. Phys.*, 2025, **27**, 9350.